Magnetism and superconductivity in underscreened Kondo chains

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We present a one dimensional model of electrons coupled to localized moments of spin $S \geq 1$ in which magnetism and superconductivity interplay in a nontrivial manner. This model has a non-Fermi liquid ground state of the chiral spin liquid type. A non-conventional odd-frequency pairing is shown to be the dominant instability of the system, together with antiferromagnetism of the local moments. We argue that this model captures the physics of the Kondo-Heisenberg spin $S = 1$ chain, in the limit of strong Kondo coupling. Finally, we discuss briefly the effect of interchain coupling.

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The interplay of magnetism and superconductivity is a fundamental problem in condensed matter physics. Superconductivity is associated with the pairing of electron states related by time reversal. Magnetic states, in which time reversal symmetry is lost, should therefore strongly compete with superconductivity. Thus it came as a surprise when it was discovered in 1984 by Schlabitz et al. [1] that magnetism and superconductivity actually coexisted in the heavy fermion compound URu_2Si_2. Since then, other heavy fermion superconductors were shown to present magnetic moments in their superconducting phase [2]. All these compounds contain rare earth or actinide ions with very localized $4f$ or $5f$ orbitals, strongly interacting with the conduction band. (This is in contrast to such cases as the Chevrel phases where magnetism and superconductivity coexist because the magnetic moments responsible for magnetism are only very weakly coupled with the electrons that form the condensate [3].)

The physics of heavy fermion compounds is believed to be described by the Kondo Lattice model in which conduction electrons interact with the local moments associated with the localized f electrons, and a large amount of theoretical work was carried out. However, although the single impurity Kondo problem is well understood [4], the theoretical analysis of the Kondo Lattice model has proven extremely difficult. This is because the Kondo effect (the quenching of the local moments) competes, in the lattice problem, with the Rudermann-Kittel-Kasuya-Yosida interaction which orders the local moments. This frustration is believed to be at the origin of the rich phase diagram of heavy fermions systems. There exist at present various theories of the superconducting ground state of the Kondo Lattice Model. Conventional scenarios involve the pairing of fermionic quasiparticles into either a spin triplet "p-wave" state or a spin singlet "d-wave" state [5]. A less conventional pairing [6] involves the formation of a spin singlet, isotropic, odd in time superconducting order parameter, known as odd-frequency pairing [7,8].

In one dimension, the theoretical situation is more favorable [9], since there are powerful methods to deal with strong interactions. Bosonization [10] and Density Matrix Renormalization Group [11] have clarified much of the physics of the single channel $S = 1/2$ Kondo lattice. One finds a paramagnetic metallic phase for small Kondo coupling and away from half filling. However, conventional superconducting fluctuations are strongly reduced [12]. Adding a direct Heisenberg interaction between the spins has been shown to cause an enhancement of odd-frequency pairing correlations. However, the formation of a spin gap precluded the observation of fluctuations towards magnetic ordering [13].

The aim of this paper is to discuss a one dimensional Kondo Lattice model with *underscreened moments* in which magnetism can be expected to dominate. We will show that in this one dimensional problem strong fluctuations to composite superconductivity coexist with strong fluctuations towards magnetic ordering.

The generalized Kondo lattice Hamiltonian in one dimension is:

$$H = -t \sum_{i,\sigma} (c^\dagger_{i,\sigma} c_{i+1,\sigma} + c^\dagger_{i+1,\sigma} c_{i,\sigma}) + \lambda_K \sum_i \vec{S}_i . c^\dagger_{i,\alpha} \vec{\sigma}_{\alpha,\beta} c_{i,\beta} + \sum_i f(\vec{S}_i \cdot \vec{S}_{i+1}) \qquad (1)$$

where $c_{i,\sigma}$ annihilates an electron, $\vec{S}_i$ is a spin-S operator, and the function f describes the spin-spin interaction. In the following, we will consider the case $\lambda_K \ll f, t$.

We shall be interested in magnetism and underscreening coexisting with superconductivity. To that purpose choose $S \geq 1$. Several forms of magnetic interaction need to be considered in this case. The simplest possibility is to take a Heisenberg coupling $f(\vec{S}_i \cdot \vec{S}_{i+1}) = \lambda_H \vec{S}_i \cdot \vec{S}_{i+1}$, but no interesting magnetic effects would ensue. We would get at $\lambda_K = 0$ either a spin gap for integer S or an effective spin 1/2 chain for half-odd integer S [14]. Turning on $\lambda_K \ll t, \lambda_H$, the case of half-odd integer S would reduce to exact screening, and a metal with a spin gap will form [15]. The case of integer S would lead to a completely trivial result, the local moments being

already completely screened by the formation of the Haldane gap preventing the Kondo effect and leaving the electrons essentially free.

Magnetic effects, on the other hand, would result from interactions in the chain, f, which lead to low energy dynamics described by effective Hamiltonians richer than the $SU(2)_1$ Wess–Zumino–Novikov–Witten (WZNW) model which govern the half-odd integer S Heisenberg [10] discussed above. We shall discuss systems with fixed points described by $SU(2)_{2S}$ ($S \geq 1$). An example is provided by the integrable spin-S chains [16–18,?], where $f = P_S = \sum_{j=1}^{S} a_j P_j$, P_j is the spin-j projector and $a_j = \sum_{i=1}^{j} i^{-1}$. Such $SU_{2S}(2)$ models arise naturally under some circumstances: it is known in particular that the Heisenberg spin-1 chain can be described as a $SU(2)_2$ WZNW model perturbed by a mass term [20] of the order of the Haldane gap. The generalization of this result to arbitrary spin S chains, based on a perturbed $SU(2)_{2S}$ WZNW model, was obtained in Ref. [21], (and will be further discussed below). Thus, our study should describe the Underscreened Kondo–Heisenberg lattice when the Kondo coupling exceeds the Haldane gap. For $S = 1$, this corresponds to $0.4\lambda_H < \lambda_K < \lambda_H$. We shall study the model away from half filling and for all S, revealing the appearance of a critical point describing a non Fermi-liquid where magnetism and superconductivity interplay [22].

We now proceed to determine the low energy behavior of the theory. Consider the Hamiltonian in the continuum limit. According to the standard prescriptions of non-abelian bosonization [10,23,24], the electrons are described by the following Hamiltonian:

$$
\begin{aligned}
H_{\rm el} &= H_\rho + H_\sigma &(2)\\
H_\rho &= \int dx \frac{v_F}{2\pi}\left[(\pi\Pi_\rho)^2 + (\partial_x\phi_\rho)^2\right] &\\
H_\sigma &= \frac{2\pi v_F}{3}\int dx(\vec{J}_R.\vec{J}_R + \vec{J}_L.\vec{J}_L) &(3)
\end{aligned}
$$

where the canonically conjugate fields Π_ρ, ϕ_ρ describe the charge excitations, and the non abelian $SU(2)_1$ currents $\vec{J}_{R,L}$ describe the electron spin excitations. The local moments are described in the low energy regime by the Hamiltonian:

$$
H_{\rm mom} = \frac{2\pi v_s}{2(1+S)}\int dx(\vec{S}_R.\vec{S}_R + \vec{S}_L.\vec{S}_L) \quad (4)
$$

where $\vec{S}_{R,L}$ are $SU(2)_{2S}$ WZNW currents. The Kondo interaction λ_K at incommensurate filling becomes:

$$
\lambda_K a \int dx(\vec{J}_R + \vec{J}_L).(\vec{S}_L + \vec{S}_R)(x) \quad (5)
$$

and preserves spin-charge separation. Carrying out standard RG calculations we find that this interaction is a combination of terms that are (marginally) relevant in the RG sense and purely marginal terms. The former drive us to a strong coupling fixed point and we need a non-perturbative way to determine it. To do so we may neglect the marginal couplings $\vec{J}_R.\vec{S}_R$ and $\vec{J}_L.\vec{S}_L$ as well as the velocity difference between electron and local moments spin excitations, and check, subsequently, their relevance at the fixed point. This leads us to the following spin Hamiltonian:

$$
\begin{aligned}
H_{\rm spin} &= H_1 + H_2 &(6)\\
H_1 &= \int dx\left[\frac{2\pi v}{2(1+S)}\vec{S}_R.\vec{S}_R + \frac{2\pi v}{3}\vec{J}_L.\vec{J}_L + \lambda_K a\vec{S}_R.\vec{J}_L\right] &\\
H_2 &= \int dx\left[\frac{2\pi v}{2(1+S)}\vec{S}_L.\vec{S}_L + \frac{2\pi v}{3}\vec{J}_R.\vec{J}_R + \lambda_K a\vec{S}_L.\vec{J}_R\right] &
\end{aligned}
$$

A similar Hamiltonian was proposed in Refs. [25,26] to describe the spin sector of a Hubbard chain coupled to N spin 1/2 chains (chain cylinder model). The $N = 2$ fixed point was analyzed in detail using an exact solution at a Toulouse point [25], and the correlation functions of the composite order parameters were obtained [26].

The fixed point Hamiltonian can be determined by arguments of *chiral stabilization* [27], since H_1 and H_2 in Eq. (6) are both chirally asymmetric (only their sum is chirally symmetric) [28]. We find, that the electron spin degrees of freedom are described by the coset CFT - $\frac{SU(2)_1 \otimes SU(2)_{2S-1}}{SU(2)_{2S}}$, or equivalently, the minimal model-M_{2S-1}, of central charge $c = 1 - \frac{6}{(2S+1)(2S+2)}$, while the local moments spin excitations are described by the $SU(2)_{2S-1}$ WZNW model:

$$
H^* = \frac{SU(2)_1 \otimes SU(2)_{2S-1}}{SU(2)_{2S}} + SU(2)_{2S-1}. \quad (7)
$$

This fixed point describes an interesting interplay of magnetism and superconductivity. We shall discuss the structure of the ground state, the thermodynamics and then the correlation functions of the model.

The ground state is a coset singlet, formed between electrons and local moments. A fraction $\frac{6}{(2S+1)(2S+2)}$ of the electron spin degrees of freedom is absorbed by the spins, leading to its complete screening. This manifests itself in the magnetic susceptibility and the specific heat:

$$
\begin{aligned}
\chi &= \frac{1}{2\pi v}(2S-1)\\
C &= \frac{\pi}{3}\left(1 + \frac{3(2S)}{2S+2} + 1 - \frac{12}{(2S+1)(2S+2)}\right)T
\end{aligned}
$$

where in the latter quantity we included also charge contributions. This leads to a Wilson ratio: $R_W = \frac{10S^2+9S-4}{(2S+1)(S+1)(2S-1)}$ going to zero as $S \to \infty$.

We now calculated the long distance behavior of the physical correlation functions. To do so we have to express the physical operators in terms of the operators around the fixed point, which we proceed to discuss. The

primary operators of $SU(2)_N$ model are $\Phi_N^{(j)}$ ($j \leq \frac{N}{2}$) and carry spin-j. The coset primaries, $\phi_{j''}^{jj'}$, ($0 \leq j \leq 1/2$, $0 \leq j' \leq S - 1/2$ and $0 \leq j'' \leq S$), are related to the $SU(2)_N$ WZNW spin-j primaries via the decomposition:

$$\Phi_{L,1}^{(j)} \Phi_{L,2S-1}^{(j')} = \sum_{|j-j'| \leq j'' \leq j+j'} \phi_{L,j''}^{j,j'} \Phi_{L,2S}^{(j'')} \tag{8}$$

The conformal weight of the coset primary is such that the two sides of the equality have the same conformal weight, implying that $\phi_{L,j''}^{jj'}$ has left conformal weight $\left(\frac{j(j+1)}{3} + \frac{j'(j'+1)}{2S+1} - \frac{j''(j''+1)}{2S+2}\right)$. Similar identities hold for the right component. Next, note that at the fixed point products of left primary operators of $SU(2)_1$ and right $SU(2)_{2S}$ WZNW models have to decompose into a sum of products of primary operators of the left minimal model and right $SU(2)_{2S-1}$ model. Moreover, the total spin has to be conserved. Therefore, one can write the decomposition:

$$\Phi_{L,1}^{(j)} \Phi_{R,2S}^{(j'')} \sim \sum_{|j-j''| \leq j' \leq j+j''} \phi_{L,j''}^{jj'} \Phi_{R,2S-1}^{(j')} \tag{9}$$

This decomposition satisfies the requirements on the indices in $\phi_{j''}^{jj'}$. It is formally similar to a Clebsch-Gordan decomposition.

Thus, at the fixed point, the spin operator is given by:

$$\vec{S}_n \sim a(\vec{S}'_R + \vec{S}'_L)(na) + \phi_{1/2}^{0,1/2} \mathrm{Tr}(\vec{\sigma} \mathrm{g}')(\mathrm{na}) \tag{10}$$

where $\vec{S}'_{R,L}$ and g' are respectively the currents and the $SU(2)$ matrix field of the $SU(2)_{2S-1}$ WZNW model, and $\phi_{1/2}^{0,1/2}$ is the field of the minimal model with scaling dimension $\frac{3}{2(2S+1)(2S+2)}$. As a result, the spin-spin correlation function behaves as:

$$\langle \vec{S}_n . \vec{S}_m \rangle \sim \frac{1}{(n-m)^2} + \frac{(-)^{n-m}}{(n-m)^{\delta_S}} \tag{11}$$

where $\delta_S = \frac{3(2S+3)}{(2S+1)(2S+2)} \ll 2$. There is a strong tendency to antiferromagnetism.

The fermion operator ψ_L, is given by:

$$\psi_L = e^{\imath(\theta_\rho + \phi_\rho)/\sqrt{2}} \phi_{L\,0}^{1/2,1/2} g'_R \tag{12}$$

where $\theta_\rho(x) = \pi \int^x \Pi_\rho(x') dx'$, $\phi_{L\,0}^{1/2,1/2}$ is the antiholomorphic component of the $\phi_0^{1/2,1/2}$ field of the minimal model, and g'_R is the holomorphic component of the g' field of the $SU(2)_{2S-1}$ WZNW model. A similar expression holds for ψ_R, in which L and R are exchanged and $\phi_\rho \to -\phi_\rho$. The resulting fermion Green's function is:

$$\langle T c_n(t) c_0^\dagger(0) \rangle \sim \frac{e^{\imath k_F na}}{(na - vt)^{1+\frac{3}{2(2S+1)}} (na + vt)^{\frac{3}{2(2S+1)}}} + \frac{e^{-\imath k_F na}}{(na + vt)^{1+\frac{3}{2(2S+1)}} (na - vt)^{\frac{3}{2(2S+1)}}} \tag{13}$$

Considering now charge density wave (CDW), spin density wave (SDW), singlet superconductor (SS) and triplet superconductor (TS) correlations, it is easy to see that they all decay with the same exponent $2 + \frac{6}{2S+1}$. These correlations are thus very strongly suppressed with respect to a free electron gas. Only for $S \to \infty$, do we recover the exponents of the free electron gas for the conventional order parameters. If we specialize to $N = 2$, we obtain the same exponents as in Ref. [25].

This leads us to investigate the presence of composite order [29,13]: the composite Charge Density Wave (c-CDW) order parameter $O_{c-CDW} = \vec{n}(x).\vec{O}_{SDW}(x)$ and the composite singlet order parameter $O_{c-S} = \vec{n}(x).\vec{O}_{TS}(x)$.

It is easy to show that the composite Charge Density Wave order parameter can be expressed at the fixed point as:

$$O_{c-CDW} \sim e^{\imath\sqrt{2}\phi_\rho} \phi_{1/2}^{1/2,0} \tag{14}$$

where the field $\phi_{1/2}^{1/2,0}$ has conformal weight $(\frac{1}{4} - \frac{3}{4(2S+2)}, \frac{1}{4} - \frac{3}{4(2S+2)})$. Similarly, for the composite singlet order, one has:

$$O_{c-S} \sim e^{\imath\sqrt{2}\theta_\rho} \phi_{1/2}^{1/2,0}. \tag{15}$$

and both correlations decay with the same exponent,

$$\langle O_{composite}(n) O_{composite}^\dagger(n') \rangle \sim \frac{1}{|n-n'|^{2-\frac{3}{2S+2}}} \tag{16}$$

Therefore, for any S, composite order parameters are dominant. This can be understood in a simple way: electrons are tightly bound to local moments, so that composite correlations, that involve coherent motion of local moments excitations and electrons, decay more slowly than conventional ones. For $S \to \infty$, conventional and composite order parameters become degenerate. This can be understood by remarking that in this limit, the local moments become classical and acquire a non-zero average so that composite and conventional order parameters become identical.

All our discussion up to now was concerned with the coupling of an integrable spin S chain with fermions. We now turn to the effect of the perturbation $\lambda \Phi_R^{(1)} \Phi_L^{(1)}$ that restores the behavior of the Heisenberg spin S chain [21]. If we assume that this term is small, i. e. that the Kondo coupling is larger than the largest gap induced by the perturbation for zero Kondo coupling, we can analyze its effect by determining whether it is relevant or irrelevant at the fixed point. The case of the spin 1 chain is special since Kac-Moody selection rules prevent the appearance of a primary operator of spin 1 in the fixed point theory. Generalizing (9) to include also non primary operators, a simple calculation shows that $\Phi_R^{(1)} \to J_R \xi'_L$, where J_R is the $SU(2)_1$ current, and ξ'_L is a Majorana fermion of

the Ising (M_1 minimal) model. This result can also be obtained from the Toulouse limit solution [25,30]. As a result, the mass term becomes a term of dimension 3 at the fixed point and is irrelevant. We therefore expect that the underscreened regime we have found will be present if λ_K exceeds the Haldane gap of the isolated spin 1 chain. For a spin $S > 1$, the operator $\Phi^{(1)}_{R,2S}$ becomes at the fixed point $\phi^{0\,1}_{L,1}\Phi^{(1)}_{R,2S-1}$. This operator has dimension $\frac{8}{2S+1} - \frac{4}{2S+2} < 2$ and is therefore *relevant* at the fixed point. It is then likely that for $S > 1$ the models that we have described flow when perturbed to the trivial Kondo-Heisenberg fixed point even for a strong Kondo coupling.

We may also examine what happens when two Kondo chains are coupled together to form a *Kondo ladder*. There are several ways to do it. One can couple the local moments of the Kondo chains by a Heisenberg coupling $\lambda_\perp \sum_i \vec{S}_{i,1}.\vec{S}_{i,2}$. At the fixed point, this gives rise to relevant terms of scaling dimension $\frac{3(2S+3)}{(2S+1)(2S+2)}$, that induce a spin gap. Second, one could consider an exchange interaction between the electrons, $\lambda_{\text{ee}} \sum_i c^\dagger_{i,\alpha,1}\vec{\sigma}_{\alpha,\beta}c_{i,\beta,1}.c^\dagger_{i,\gamma,2}\vec{\sigma}_{\gamma,\delta}c_{i,\delta,2}$. It is easily seen that such an interaction only leads to irrelevant terms, and does not affect our fixed point. Finally, one could consider interchain hopping of the electrons $t_\perp \sum_i (c^\dagger_{i,\sigma,1}c_{i,\sigma,2} + \text{h. c.})$. At the fixed point, this leads to an operator of dimension $1 + \frac{3}{2S+1}$, relevant for $S \geq 3/2$. For $S = 1$, this term is marginal but it generates a relevant RKKY interaction between the local moments that destabilizes the chiral fixed point.

We have obtained a physical picture of the one-dimensional underscreened Kondo Lattice. The formation of a chiral non-Fermi Liquid results in strong antiferromagnetic fluctuations accompanied with composite pairing. This picture is reminiscent of the situation that obtains in three dimensional heavy fermion systems [2]. It would be very worthwhile to try to determine if some analog of a chiral non-Fermi liquid can be found in higher dimensional Kondo Lattice models. A good starting point would be an array of Kondo-underscreened chains coupled by interchain hopping.

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